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* SUPPORTING INFORMATIN B
* This file contains Polymer & Electrolyte Transferable Force Field (PET-FF)
PET-FFver2.0
* Any line starting with "*" is a comment line
*
* This file could be used with the SystemGenerator.exe program to create input
* files for the Lucretius (MD) program and Lucretius-based force field (FF)
fitting program.
* SystemGenerator.exe uses this file and cartesian coordinates (*.cc1 or *.xyz)
files for create ff.dat, connectivity.dat,coords.dat and *.h files
*
* The repulsion-dispersion (RD) atom types and atomic charges are determined
* based upon atom label and labels of atoms it is connected to.
* Bond, bend, torsional and out-of-plane deformation types
* are determined based upon RD and charge types of contitutive atoms.
*
* Below is the list of systems that the force field has been tested upon
* C2H6, C10H22, C13H28, C2F6, C6F14, C20F44, ether, DME, diglyme, triglyme,
* (PEO, PPO, PTMO, glymes, EC , PC, DMC, GBL doped LiTFSI), SO2, DMA
*
* The following "special" atom types (labels) can be used (in *.cc1 or *.xyz
files)
* Lp is the extended charge to approximate a lone pair
* Oc  - carbonyl oxygen
* Oec - ether oxygen next to carbonyl group
* Ocd - carbonyl oxygen in (Ocd)2-Ccl-O-R groups (EDC, MMC) having charge -1
* Ccl - carbonyl carbon in linear carbonates (DMC,DMK)
* Ccc - carbonyl carbon in cyclic carbonates (EC,PC,GBL)
* Lp  - extended charge (combined lone-pair) at ether oxygen
* Lp1 - special extended charge (combined lone-pair) in oxymethylene oxides
* Oh  - hydroxyde oxygen
* Hh  - hydroxyde hydrogen
* CU  - united atom carbon
* Next line lists valid input atom types and should be terminated with "!"
 H  Hh  Li   B   C  Ccl Ccc  N   O  Oc  Oec Ocd  Oh  F   S   Si Lp  Lp1  K  CU !
* Van der Waals radii for atoms(in A) are used to find bonds using arithmetic
comb. rules
1.1 1.1 0.0 1.5 1.8 1.6 1.6 1.5 1.6 1.6 1.6 1.6 1.6 1.6 2.4 1.8 0.6 0.6 0.0 1.8
* Number of Repulsion-Dispersion (RD) ATOM TYPES used in this force field
 18
* Each atomtype is defined by the number of atoms it is connected to and their
types
* Use X to define any input atom type
* Format:RDType (repulsion-dispersion type) on a separate line, a
label(3char),atom mass, the number of charge types listed
* ChargeType definition: (Charge type number),
AtomType,MM2index(optional,0=="any"),Number of Bonds, Bonded Atom
Labels,Q(charge),Polarization, comments
RDType C    12.011  21    ! transferable carbon (except CH3- ethers,carbony
group)
1   C   0  4  H   H   H   H   -0.4400  0.91  ! C*H4
2   C   0  4  C   H   H   H   -0.3300  0.91  ! C-(C)*H3
3   C   0  4  C   C   H   H   -0.2200  0.91  ! C-(C)*H2-C
4   C   0  4  C   C   C   H   -0.1100  0.91  ! in branched alkanes,C-C*(CH)-C
(PTMO-comb)
5   C   0  4  F   F   F   F    0.4704  0.60  ! C*F4
6   C   0  4  C   F   F   F    0.3528  0.60  ! C-(C)*F3
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7   C   0  4  C   C   F   F    0.2352  0.60  ! C-(C)*F2-c
8   C   0  4  C   C   C   F    0.1176  0.60  ! in branched fluoro alkanes
9   C   0  4  S   F   F   F    0.2988  0.60  ! (F)3-C*-S in TFSI-
10  C   0  4  S   C   F   F    0.1812  0.60  ! S-C*(F2)-C in TFSI-ether
11  C   0  4  O   C   H   H   -0.1887  0.50  ! O-C*(H2)-C (in PEO)
12  C   0  4  N   H   H   H   -0.2300  0.91  ! H3(C*)-N in dimethyl amine
13  C   0  4  O   O   H   H   -0.1574  0.60  ! O-C*(H2)-O (POM)
14  C   0  4  O   C   C   H   -0.0787  0.50  ! C-(C)*HCC in comb-branched
ethers, PPO
15  C   0  4  Oec C   H   H   -0.0561  0.50  ! Oec-C*(H2)-C(H2) (EC,PC,GBL)
16  C   0  4  Oec C   C   H    0.0539  0.60  ! Oec-C*(H,CH2)-CH3 (PC)
17  C   0  4  Ccl H   H   H   -0.3908  0.91  ! in acetone (DMK)
18  C   0  0                   0.0000  0.00  ! blank
19  C   0  4  Ccc C   H   H   -0.1847  0.50  ! (CH2-C*(H2)-Ccc) GBL
20  C   0  0                   0.0000  0.00  ! blank
21  Ccl 0  4  Oc  Ccl H   H   -0.1750  0.50  ! ethylene dicarbonate (alkyl
carbonate), EDC
RDType Cm   12.011  2     ! O-CH3 in ethers, linear carbonates
1   C   0  4  O   H   H   H   -0.2987  0.50  ! O-C*H3 (terminal group in ethers)
2   C   0  4  Oec H   H   H   -0.1461  0.50  ! O-C*H3 in DMC, MMC?
RDType Cc   12.011  5     ! in carbonyl groups (except)
1   Ccc 0  3  Oc   Oec Oec     0.5977  0.26  ! Oec-(C*=Oc)-Oec in EC,PC
2   Ccl 0  3  Oc   Oec Oec     0.3737  0.26  ! Oec-(C*=Oc)-Oec in DMC
3   Ccl 0  3  Ocd  Ocd Ocd     0.5828  0.26  ! O-(C*=O)-O in ethylene
dicarbonate (EDC,MMC)
4   Ccc 0  3  Oc   Oec  C      0.5071  0.26  ! CH2-C*(=O)-O(Lp) GBL
5   Ccl 0  3  C    Oc   C      0.6087  0.26  ! DMK (acetone) CH3-C*(Oc)-CH3
RDType O   15.999  11
1   Oec 0  3  Ccl C   Lp       0.0854  0.93  ! Ccl-O*(Lp)-C(H2) in linear
carbonates(DMC)
2   O   0  3  C   C   Lp       0.1500  1.25  ! O-Lp in PEO
3   Oc  0  1  Ccc             -0.4871  1.53  ! O*=C(sp2)(EC,PC) GBL(pol=1.4)
4   Oec 0  3  Ccc C   Lp      -0.0066  0.90  ! Ccc-Oec(Lp)*-C(H2) (EC,PC,GBL)
5   O   0  1  S               -0.3588  1.70  ! O(TFSI,SO2),for SO2 use 1.050 A^3
polariz.
6   O   0  3  C   C   Lp1      0.2326  1.27  ! O-Lp in POM
7   Oc  0  1  Ccl             -0.4871  1.40  ! O*=C(sp2)in (DMC),pol(DMK)=1.35
8   Oec 0  0                   0.0     0.0   ! blank
9   Oc  0  0                   0.0     0.0   ! blank
10  Oc  0  3  Ccl  C  Lp      -0.0306  0.70  ! C(carbonyl)-O*-C(ether) ethylene
dicarbonate:EDC
11  Ocd 0  1  Ccl             -0.6923  1.30  ! O*=C(sp2) ethylene
dicarbonate:EDC
RDType S  32.066   2
1   S   0  4  O   O   C   N    0.4845  1.00  ! S in TFSI-
2   S   0  3  O   O   Lp       1.0442  0.900 ! S in SO2
RDType Lp  0.00   5
1   Lp  0  1  O               -0.2126  0.00  ! Extended charge to approximate
Lone Pair (PEO)
2   Lp  0  1  Oec             -0.2126  0.00  ! Extended charge to approximate
Lone Pair (EC,PC,DMC,GBL,EDC)
3   Lp  0  1  S               -0.3266  0.55  ! Extended charge in SO2
4   Lp  0  1  N               -0.0000  0.00  ! Extended charge next N in TFSI
5   Lp1 0  1  O               -0.2952  0.00  ! POM
RDType H   1.008  4   ! all H
1   H   0  1  C                0.1100  0.46  ! H bonded to any C
2   H   0  0                   0.1100  0.46  ! blank
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3   H   0  1  O                0.0657  0.00  ! H on SiO2 surface
4   H   0  1  N                0.3000  0.46  ! H on SiO2 surface
RDType Li  6.941  1
1   Li  0  0                   1.0000  0.00  ! Li+ ion
RDType F   18.998  2
1    F  0  1  C               -0.1176  0.56  ! in TFSI and PTFE
2    F  0  1  B                0.2680  0.89  ! in TFSI and PTFE
RDType N   14.007  2
1   N   0  2   S   S          -0.4258  1.56  ! in TFSI (set)
2   N   0  3   C   C   H      -0.5000  1.56  ! in dimethyl amine from Dyksra
RDType B   8.298  1
1   B   0  4   F   F   F   F  -1.0720  0.00  ! in TFSI
RDType Si  28.086  6
1   Si  0  4   O   C   C   C   0.0     0.0  ! Si-end group(CH3)
2   Si  0  4   O   O   C   C   0.0     0.0
3   Si  0  4   O   H   H   H   0.0     0.0  ! Si-end group(H3)
4   Si  0  4   O   O   O   O   0.5236  0.0  ! in the middle of SiO2
particle(3oxygens)
5   Si  0  3   O   O   O       0.3927  0.0  ! bonded to 3 oxygens
6   Si  0  2   O   O           0.2618  0.0  ! bonded to 2 oxygens
RDType OSi 15.999   3
1   O   0  2  Si  Si          -0.2618  0.0  ! in the middle of SiO2 particle
2   O   0  1  Si              -0.1309  0.0  ! singly bonded to Si
3   O   0  2  Si  H           -0.1966  0.0  ! on SiO2 surface next to H
RDType Cg  12.011   1         ! graphite carbone
1   C   0  3  C    C  C        -0.00   0.00  ! C (graphite)
RDType K  39.1   1            !  K+
1   K   0  0                    1.00   0.73  ! K+
RDType Oh  15.999  1
1   Oh  0  1  Hh              -1.2000  1.27  ! Oh
RDType Hh  1.008   1    ! all Hh
1   Hh  0  1  Oh               0.2000  0.46  ! Hh
RDType CU    12.011  4    ! united atom carbon
1   CU  0  3  CU  CU  CU      -0.0000  0.00  ! CU-CU*(CU)-CU
2   CU  0  2  CU  CU          -0.0000  0.00  ! CU-CU*-CU
3   CU  0  2  CU  C           -0.0000  0.00  ! CU-CU*-C
4   CU  0  1  CU              -0.0000  0.00  ! CU*-CU
*
* REPULSION and DISPERSION parameters: SELF-TERMS A,B,C
* Next line:Format of nonbonded parameters "ABC" coefficients or "R_E" standing
for R*,epsilon(and lamda)
ABC
*
* Self-terms should always be defined first to allow calculation of default
cross-terms
* A,B,C (R*,epsilon,lamda) [exp-6,lj9-6, lj126 parameters could be used]
*
Li        44195.0   7.2770     1.06   exp-6  ! for Li+
B        104830.0   3.5398   693.24   exp-6  ! B from DREIDING (interpolation)
H         15480.0   4.8165    29.46   exp-6  ! H connected to carbon
C        165734.9   3.8867   332.40   exp-6  ! -C*(H2)- sp3 transferable carbon
Cm       165734.9   3.8867   375.00   exp-6  ! C*(H3)-O
Cc        39080.0   3.9000   500.00   exp-6  ! carbonyl carbon (EC,PC,DMC,GBL)
O         48833.0   3.8236   310.00   exp-6  ! generic oxygen (ether,
carbonates,SO2,TFSI-)
Oh        23473.0   3.3000   310.00   exp-6  ! generic oxygen (ether,
carbonates,SO2,TFSI-)
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N         26800.0   3.4050   620.00   exp-6  ! fitted to DNA dimer GDS FF C
Lp            1.0   0.0000   000.00   lj126  ! lone-pair
F          9693.8   3.5861   164.20   exp-6  ! F-(C) from C6F14 fit
S         95900.0   3.4013  1304.00   exp-6  ! S=(O)2 fitted to SO2 properties
Cg       165734.9   3.8867   332.40   exp-6  ! approximate Cg in graphite, the
same as -C*(H2)-
K        538554.6   4.0200   970.00   exp-6  ! K+ (to be fitted)
Hh         3100.0   4.0000     5.0    exp-6  ! Hh (fit to OH rotation to in OH-
/DME)
CU       165734.9   3.8867   332.40   exp-6  ! united atom carbon
*
* REPULSION and DISPERSION parameters: CROSS-TERMS A,B,C (two labels are
required)
* Self-terms should should have been defined above to allow calculation of
default cross-terms
*
Li  H    37404.5    5.3341     5.59    exp-6
Li  Cm   95861.2    4.3460    19.94    exp-6
Li  C    95861.2    4.3460    18.77    exp-6
Li  Cc   95861.2    4.3460    23.02    exp-6
Li  N    15700.0    3.6717    25.64    exp-6
Li  O    49530.0    4.4757    18.13    exp-6
Li  F    32368.0    4.8200    13.19    exp-6
Li  S    48196.0    3.4800    37.18    exp-6
Li  CU   95861.2    4.3460    18.77    exp-6
Lp  Li       0.1    0.0        0.00    lj126
Lp  H        0.1    0.0        0.00    lj126
Lp  C        0.1    0.0        0.00    lj126
Lp  Cm       0.1    0.0        0.00    lj126
Lp  Cc       0.1    0.0        0.00    lj126
Lp  O        0.1    0.0        0.00    lj126
Lp  Oh       0.1    0.0        0.00    lj126
Lp  N        0.1    0.0        0.00    lj126
Lp  F        0.1    0.0        0.00    lj126
Lp  S        0.1    0.0        0.00    lj126
Lp  K        0.1    0.0        0.00    lj126
Lp  Hh       0.1    0.0        0.00    lj126
Li  Cg    1000.0    4.3460     0.00    exp-6
Lp  CU       0.1    0.0        0.00    lj126
O   Hh       0.0    0.0        0.00    exp-6
*
* BONDS are defined using
* RDtype1,charge1, RDtype2,charge2, K, R0, R0-constrained
* use "0" to specify any charge type in definition of bonds, bends, torsions
* Important definition of generic type should preceed the specific types
C   0  C   0   618.0  1.53    1.53    ! fitted to b3lyp/aug-cc-pvdz(C4H10)
C   11 C   11  618.0  1.516   1.516   ! PEO (b3lyp/aug-cc-pvDz DME ttt, tgt,
tg+g-)
C   2  C   11  618.0  1.516   1.516   ! methyl-ethyl-ether (the same as PEO C-C
bond)
C   2  C   14  618.0  1.531   1.531   ! C*(H3)-C* in PPO
C   14 C   11  618.0  1.516   1.516   ! PPO (transfered from PEO)
C   15 C   15  618.0  1.533   1.533   ! EC: Oec-C*(H2)-C*(H2)-Oec
C   16 C   2   618.0  1.516   1.516   ! PC: C(H3)-C fitted
C   6  C   7   618.0  1.560   1.560   ! PTFE CF3-CF2-
C   7  C   7   618.0  1.560   1.570   ! PTFE -CF2-CF2-
C   6  C   6   618.0  1.560   1.560   ! PTFE CF3-CF3
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C   0  H   0   655.0  1.10    1.10    ! fitted to b3lyp/aug-cc-pvdz(C2H4,C4H10)
C   0  O   0   739.0  1.419   1.419   ! generic PEO (b3lyp/aug-cc-pvDz DME ttt,
tgt, tg+g-)
C   11 O   2   739.0  1.419   1.419   ! PEO (b3lyp/aug-cc-pvDz DME ttt,
tgt,tg+g-)
C   15 O   4   739.0  1.440   1.440   ! EC C-C*(H2)-Oec*(Lp)-C (also PC)
C   16 O   4   739.0  1.450   1.450   ! PC C-C*(H2)-Oec*(Lp)-C (fitted)
Cc  0  O   0  1368.0  1.200   1.200   ! generic carbonyl Cc=Oc bond fitted to EC
+ DMC
Cc  2  O   7  1368.0  1.200   1.200   ! DMC Oc=Ccl (from combined EC, DMC fit)
Cc  1  O   3  1368.0  1.200   1.200   ! EC: Oec-Ccc (from combined EC, DMC fit)
Cc  1  O   4   739.0  1.35    1.35    ! EC: Oc=Ccc (from combined EC, DMC fit)
Cc  2  O   1   739.0  1.363   1.363   ! DMC Cc*(O3)-O*(Lp)-R
C  17  Cc  5   739.0  1.52    1.52    ! DMK, Ccl-C fitted
Cc  4  C  19   900.0  1.53    1.53    ! GBL O=C*(OLp)-CH2  (same as generic C-C)
Cc  4  O   3  1368.0  1.21    1.21    ! GBL *O=C*(OLp)
Cc  4  O   4   900.0  1.38    1.38    ! GBL O=C*(OLp)-O*(Lp)
C   15 O   4   739.0  1.45    1.45    ! GBL C-C*(H2)-O*(Lp)-C
Cc  5  O   7  1368.0  1.22    1.22    ! DMK *O=C*(OLp) fitted
O   0  Lp  0     0.0  0.50    0.50    ! extended charge to approximate lone pair
Cm  0  H   0   655.0  1.10    1.10    ! fitted to b3lyp/aug-cc-pvdz(C2H4,C4H10),
assumed constrained
Cm  2  H   0   655.0  1.10    1.10    ! DMC (transfered from alkanes)
Cm  0  O   0   739.0  1.415   1.415   ! generic from PEO (b3lyp/aug-cc-pvDz DME
ttt, tgt)
Cm  1  O   2   739.0  1.415   1.415   ! PEO (b3lyp/aug-cc-pvDz DME ttt, tgt)
Cm  2  O   1   739.0  1.440   1.440   ! DMC (fitted to DMC)
F   0  C   0   722.0  1.340   1.340   ! C*-F3 in PTFE and TFSI-
F   1  C   6   722.0  1.339   1.341   ! C*-F3 in PTFE
F   1  C   7   722.0  1.351   1.355   ! C*-F3 in PTFE
C   0  S   0   596.0  1.902   1.902   ! TFSI-
S   0  O   0  1656.0  1.484   1.484   ! TFSI-
S   0  N   0   974.0  1.633   1.633   ! TFSI-
N   0  Lp  0     0.0  0.5     0.5     ! extended charge in TFSI- (not used)
S   0  Lp  0     0.0  0.5     0.5     ! S-Lp, distance from S to the extended
charge in SO2
N   0  C   0   734.0  1.460   1.460   ! in CH3-NH-CH3
N   0  H   0   720.0  1.016   1.016   ! in CH3-NH-CH3 (from Estane)
Cg  0  Cg  0   618.0  1.420   1.420   ! Cg-Cg bond in graphite
Oh  1  Hh  1   900.0  0.97    0.97    ! Oh-Hh bond
O  11  Cc  2   900.0  1.252   1.252   ! Ocd=Ccl alkyl carbonates: EDC, MMC
O  10  Cc  2   900.0  1.436   1.436   ! Ccd-EO  alkyl carbonates: EDC, MMC
O  10  C  21   900.0  1.427   1.427   ! EO-C(H2) alkyl carbonates: EDC, MMC
C  21  C  21   618.0  1.528   1.528   ! EO-CH2-C(H2)-EO alkyl carbonates: EDC,
MMC taken from PEO
CU  0  CU  0   618.0  1.53    1.53    ! CU-CU
CU  0  C   0   618.0  1.53    1.53    ! CU-CU
*
* BENDS !!! Generic type should preceed the specific type
* RDtype1,charge1, RDtype1,charge1, RDtype3,charge3, K, theta0
*
C   0  C   0  C   0      108.00     112.2 ! Generic C-C-C
C  11  C   14 C   2      108.00     112.2 ! 1,2-dimethoxy propane
C  11  C   3  C   11     108.00     112.2 ! PTMO (fitted to 1,3-DMP)
C  11  C   14 C   11     108.00     112.2 ! PEO-Comb
C   2  C   3  C   2      108.00     114.4 ! b3lyp/Dz,alkanes (c4h10 trans, c5h12
tt)
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C   2  C   3  C   3      108.00     114.4 ! b3lyp/Dz,alkanes (c4h10 trans, c5h12
tt)
C   3  C   3  C   3      108.00     114.4 ! b3lyp/Dz,alkanes (c4h10 trans, c5h12
tt)
C   6  C   7  C   7      160.60     115.6 ! PTFE
C   7  C   7  C   7      160.60     115.6 ! PTFE
C   2  C   16 C   15     108.00     114.2 ! PC (fitted)
Cc  4  C   19 C   3      184.00     103.1 ! Cc-C-C GBL k- J.Phys.Chem. B 2004,
109, 17992
C  19  C   3  C   15     184.00     102.7 ! C-C-C GBL k- J.Phys.Chem. B 2004,
109, 17992
H   0  C   0  C   0       86.00     110.0 ! generic H-C-C, all ethers
H   0  C   11 C   11      86.00     110.0 ! PEO (DME b3lyp/Dz)
H   0  C   2  C   3       86.00     110.5 ! from C4,C5 alkanes
H   0  C   3  C   3       86.00     110.5 ! from C4,C5 alkanes
H   0  C   3  C   2       86.00     110.5 ! from C4,C5 alkanes
H   0  C   19 Cc  4       95.7      108.8 ! H-C-Cc GBL k- J.Phys.Chem. B 2004,
109, 17992
H   0  C   0  H   0       77.00     108.2 ! in alkanes, polyethers
H   0  C   2  H   0       77.00     107.7 ! in the terminal group alkanes
H   0  Cm  0  H   0       77.00     109.3 ! in the terminal group ethers
H   0  Cm  1  H   0       77.00     109.3 ! PEO, for CH3 termination
H   0  C   15 H   0       77.00     109.6 ! H-C-H in EC, different from PE, PEO
H   0  Cm  0  O   0      112.00     109.3 ! generic from PEO
H   0  Cm  1  O   2      112.00     109.3 ! PEO
H   0  Cm  2  O   1      112.00     107.9 ! DMC:H-Cm-Oec (fitted)
H   0  C   0  O   0      112.00     110.0 ! generic H-C -O from PEO
H   0  C   11 O   2      112.00     110.0 ! PEO
H   0  C   13 O   0      112.00     104.6 ! POM (1,3-DDE-gggg,b3lyp/Dz)
H   0  C   14 O   2      112.00     110.0 ! PEO-Comb (fitted)
H   0  C   15 O   4      112.00     108.5 ! H-C-Oec fitted to EC, different from
PEO
H   0  C   16 O   4      112.00     106.8 ! H-C-EO fitted to PC
C   0  C   0  O   0      172.00     110.0 ! generic from PEO
C   11 C   11 O   2      172.00     110.0 ! PEO
C   2  C   11 O   2      172.00     110.0 ! methyethyl ether (using DME value)
C   11 C   14 O   2      172.00     110.0 ! PPO (1,2-DMP ggt)
C   2  C   14 O   2      172.00     110.0 ! PPO (1,2-DMP ggt)
C   11 C   14 O   2      172.00     110.0 ! PEO-comb (1,2-DMP ggt)
C   14 C   11 O   2      172.00     110.0 ! PPO,PEO-comb (checked on 1,2-DMP
ggt)
C   3  C   11 O   2      172.00     110.0 ! PTMO (fitted to 1,3 DMP)
C   15 C   15 O   4      220.00     108.7 ! C-C-Oec EC  (fitted)
C   19 Cc  4  O   4      202.00     110.3 ! C-Cc-Obl GBL Kbend-J.Phys.Chem. B
2004, 109, 17992
C   19 Cc  4  O   3       89.90     131.0 ! C-Cc-Oc  GBL Kbend-J.Phys.Chem. B
2004, 109, 17992
C   3  C   15 O   4      141.00     106.6 ! C-C-Obl  GBL Kbend-J.Phys.Chem. B
2004, 109, 17992
Cm  0  O   0  Cm  0      149.00     110.0 ! generic, transfered from 1,2-DME
Cm  1  O   2  Cm  1      149.00     110.0 ! PEO
Cm  0  O   0  C   0      149.00     110.0 ! PEO, generic Cm-O-C
Cm  1  O   2  C   11     149.00     110.0 ! PEO
C   0  O   0  C   0      149.00     108.8 ! PEO,PPO, PEO-comb generic C-O-C
(from DME fit)
C  11  O   2  C   11     149.00     108.8 ! PEO
C  14  O   2  C   11     149.00     108.8 ! PPO
```

```
O   4  Cc  0  O   0      280.00     112.2 ! generic from EC Oec-Cc-Oec
O   4  Cc  1  O   4      280.00     112.2 ! Oec-Cc-Oec EC (fitted),fc from Masia
et al on EC
O   1  Cc  2  O   1      280.00     109.3 ! DMC:Oec-Cc-Oec (fitted),fc from
Masia et al on EC
O   7  Cc  2  O   1      140.00     125.3 ! DMC:Oc-Cc-Oec (fitted),fc from Masia
et al on EC,GBL
O   3  Cc  0  O   3      140.00     123.9 ! generic from Oec-Cc=Oc EC
O   4  Cc  1  O   3      140.00     123.9 ! Oec-Cc=Oc EC (fitted)
O   3  Cc  4  O   4      190.4      122.6 ! Oc-Cc-Obl  GBL k- J.Phys.Chem. B
2004, 109, 17992
O   0  Cc  0  O   0      130.00     124.7 ! generic
C   0  O   0  Cc  0      200.00     113.2 ! generic C-Oec-Cc from EC
C   15 O   4  Cc  1      200.00     113.2 ! C-Oec-Ccc EC (fitted),fc from Masia
et al on EC,GBL
C   16 O   4  Cc  1      200.00     113.2 ! PC: C-Oec-Ccc from EC
C   15 O   4  Cc  4      200.00     109.1 ! GBL, C-Oec-Ccc fitted
C   15 C   15 H   0       86.00     112.3 ! C-C-H in EC (fitted), different from
as in PE, PEO
C   16 C   15 H   0       86.00     110.7 ! C-C-H in PC, different from PE, PEO
C   15 C   16 H   0       86.00     112.3 ! C-C-H in PC, different from PE, PEO
O   0  C   13 O   0      144.0      108.6 ! POM (DMDME-gggg,b3lyp/Dz)
Cm  0  O   0  Cc  0      200.00     110.9 ! generic (fitted to DMC)
Cm  2  O   1  Cc  2      200.00     110.9 ! DMC (fitted),fc from Masia et al on
EC,GBL
F   0  C   0  F   0      240.00     110.3 ! PTFE, change fc to 124
F   0  C   6  F   0      240.00     109.1 ! PTFE, change fc to 124
F   0  C   0  C   0      180.00     109.0 ! PTFE
O   0  S   0  O   0      191.00     120.0 ! TFSI
S   0  N   0  S   0      175.00     124.3 ! TFSI
O   0  S   0  N   0      208.00     114.0 ! TFSI
C   0  S   0  N   0      210.00     102.3 ! TFSI
O   0  S   0  C   0      204.00     103.1 ! TFSI
F   0  C   0  S   0      130.00     109.5 ! TFSI
F   0  C   9  F   0      124.00     109.0 ! TFSI, TFSIether
C  10  C   11 H   0       86.00     109.2 ! TFSIether
F   0  C   10 F   0      124.00     109.0 ! TFSIether
C  11  C   10 S   0      180.00     112.7 ! TFSIether (fitted to TFSIether)
C  10  C   11 O   0      172.00     109.6 ! TFSIether (fitted to TFSIether)
F   0  C   10 C   11     180.00     111.8 ! TFSIether (fitted to TFSIether)
C   0  Cc  5  C   0      126.00     121.8 ! DMK fitted b3lyp/Dz, Kbend from
AMBER
O   0  Cc  5  C   0      160.00     116.4 ! DMK fitted b3lyp/Dz, Kbend from
AMBER
H   0  C   17 Cc  5       86.00     110.5 ! DMK, from alkanes (checked on DMK)
H   0  N   0  C   0       86.00     106.9 ! in CH3-HN-CH3 (from Estane)
C   0  N   0  C   0      100.00     110.9 ! in CH3-HN-CH3 (fc from AMBER)
H   0  C   0  N   0      100.00     109.9 ! in CH3-HN-CH3 (fc from AMBER)
Cg  0  Cg  0  Cg  0      100.00     120.0 ! Cg-Cg-Cg bend in graphite
O  11  Cc  2  O   11     190.4      132.8 ! Oc-C1-Oc Kb from GBL, alkyl
carbonates: EDC,MMC
O  11  Cc  2  O   10     190.4      113.6 ! Oc-C1-Oc Kb from GBL, alkyl
carbonates: EDC,MMC
Cc  2  O   10 C   21     142.00     110.0 ! Cc-EO-C  Kb in GBL, alkyl
carbonates: EDC,MMC
C  21  C   21 O   10     172.00     106.8 ! taken from PEO: alkyl carbonates:
EDC,MMC
```

```
CU  0  CU  0  CU  0       36.00     112.2 ! CU-CU-CU
CU  0  CU  0  C   0       36.00     112.2 ! CU-CU-CU
CU  0  C   0  C   0      108.00     112.2 ! CU-CU-CU
*
* TORSIONS !!! Generic type should preceed the specific type
* iat,jat,kat,jat types; #folds; constants -1/2Kn*cos(fi*n)
*
H   0  C   0  C   0  C   0     3  0.000    0.000   -0.300
H   0  C   0  C   0  H   0     3  0.000    0.000   -0.300
C   0  C   0  C   0  C   0     4  0.060    0.132    0.060  -0.429    ! alkanes
H   0  C   0  C   0  O   0     3  0.000    0.000   -0.300            ! PEO, PTMO
H   0  Cm  0  O   0  Cm  0     3  0.000    0.000   -0.600            ! PEO
H   0  C   0  O   0  Cm  0     3  0.000    0.000   -0.600            ! PEO
H   0  C   0  O   0  C   0     3  0.000    0.000   -0.600            ! PEO
H   0  Cm  0  O   0  C   0     3  0.000    0.000   -0.600            ! PEO
Cm  0  O   0  C   0  C   0     4  2.710    0.725   -0.500  -0.260    ! generic
C-O-C-C from ME-ether fit
C   0  O   0  C   0  C   0     4  2.710    0.725   -0.500  -0.260    ! generic
C-O-C-C from ME-ether fit
Cm  0  O   2  C   11 C   11    4  3.380    0.927    0.020  -0.155    ! PEO
(fitted to DME)
C  11  O   2  C   11 C   11    4  3.380    0.927    0.020  -0.155    ! PEO
(fitted to DME)
C  11  O   2  C   14 C   11    4  1.720    0.134   -0.500  -0.270    ! PEO-comb
C  11  O   2  C   14 C   2     4  1.720    0.134   -0.500  -0.270    ! PPO
C  14  O   2  C   11 C   14    4  2.820    0.940    0.812  -0.456    ! PPO  C*-
O-C-C*
Cm  0  O   2  C   14 C   11    4  1.720    0.134   -0.500  -0.270    ! PEO-comb
Cm  0  O   2  C   14 C   2     4  1.720    0.134   -0.500  -0.270    ! PPO
Cm  0  O   2  C   11 C   14    4  1.720    0.134   -0.500  -0.270    ! PPO
O   0  C   0  C   0  O   0     4 -0.600   -2.146   -0.220  -0.240    !
PEO,PPO,PEO-comb(fitted to DME)
O   2  C   0  C   0  C   0     4  0.713   -0.685    0.130  -0.300    ! generic
for ethers, from PTMO:1,3-DMP
O   2  C   11 C   3  C   11    4  0.713   -0.685    0.130  -0.300    ! in
PTMO:1,3-DMP
O   2  C   11 C   14 C   11    4  0.982   -1.144   -0.400   0.276    ! PPO, DMD,
1,2-DMP
O   2  C   11 C   14 C   2     4  0.982   -1.144   -0.400   0.276    ! PEO-comb
using PPO parameters
Cm  0  O   0  C   0  O   0     4  1.198   -2.598   -1.339   -0.610    ! POM
C   0  O   0  C   0  O   0     4  1.198   -2.598   -1.339   -0.610    ! POM
O   4  C   15 C   15 O   4     3  0.000  -17.000    5.460            ! EC
(fitted)
C   15 C   15 O   4  Cc  1     0  0.000                              ! EC (set
to zero)
O   1  Cc  0  O   0  Cm  0     2  1.29     11.61                     ! Oec-Cc-
Oec-C generic from DMC
O   1  Cc  2  O   1  Cm  2     2  1.29     11.61                     ! DMC
(fitted)
Cc  2  O   1  Cm  2  H   0     3  0.000    0.000   -0.600            ! DMC
(transfered from PEO)
H   0  C   0  O   0  Cc  0     3  0.000    0.000   -0.600            ! EC,PC
from PEO
C   16 C   15 O   4  Cc  1     0  0.000                              ! PC set to
zero
```

```
C   15 C   16 O   4  Cc  1     0  0.000                              ! PC set to
zero
C   2  C   16 O   4  Cc  1     0  0.000                              ! PC set to
zero
C   2  C   16 C   15 O   4     0  0.000                              ! PC set to
zero
O   4  C   16 C   15 O   4     2  0.000   -4.740                      ! PC
(fitted)
C   0  S   0  N   0  S   0     3 -5.600   -5.090   -1.356             ! TFSI
F   0  C   0  S   0  O   0     0  0.000
F   0  C   0  S   0  N   0     3  0.000    0.000   -0.400             !
TFSI,TFSIether
F   0  C   0  C   0  O   0     1  0.000                              ! TFSIether
S   0  C   10 C   11 O   0     3  0.800   -0.500   -0.000            ! TFSIether
(fi2)
H   0  C   11 C   10 F   0     0                                     ! TFSIether
H   0  C   11 C   10 S   0     0                                     ! TFSIether
C   11 C   10 S   0  N   0     4 -0.380   -0.122   -0.300  -0.383    ! TFSIether
(fi3)
O   5  S   0  C   0  C   0     0  0.000                              ! TFSIether
C   11 O   0  C   11 C   10    4  1.116   -1.401    0.402   0.258    ! TFSIether
(fi1)
Cm  0  O   0  C   11 C   10    4  1.116   -1.401    0.402   0.258    ! TFSIether
(fi1 in the fit)
O   5  S   0  N   0  S   0     0  0.000
H   0  C   17 Cc  5  C   17    3  0.000    0.000   -0.300             ! DMK
(acetone) from alkane
H   0  C   17 Cc  5  O   7     3  0.000    0.000    0.060             ! DMK
(acetone) from alkane
H   0  C   17 C   18 O   0     3  0.000    0.000   -0.045            ! fitted to
CH3-rotation
C   0  C   7  C   7  C   0     7 -1.463   -0.722    1.413  -1.145 -0.220  0.000
0.761 !PTFE
F   0  C   0  C   0  C   0     0                                      ! PTFE
F   0  C   0  C   0  F   0     3  0.000    0.000   -0.480             ! PTFE
H   0  C   0  N   0  C   0     3  0.000    0.000   -0.620             ! DMA
(taken from H-C -O-C  PEO)
O   3  Cc  4  O   4  C   15    0  0.000                              ! Oc-Cc-EO-
C GBL
O   3  Cc  4  C   19 C   3     0  0.000                              ! Oc-Cc-C-C
GBL
O   3  Cc  4  C   19 H   0     0  0.000                              ! Oc-Cc-C-H
GBL
O   4  Cc  4  C   19 H   0     0  0.000                              ! EO-Cc-C-H
GBL
Cc  4  C   19 C   3  C   15    0  0.000                               ! Cc-C-C-C
GBL
Cc  4  C   19 C   3  H   0     0  0.000                               ! Cc-C-C-H
GBL
C   19 Cc  4  O   4  C   0     0  0.000                              ! Oc-Cc-EO-
C GBL
C   19 C   3  C   15 O   4     3  0.000     9.100    -4.00           ! C-C-C-EO
GBL
C   3  C   19 Cc  4  O   4     0  0.000                              ! C-C-Cc-EO
GBL
Cc  4  O   4  C   15 C   3     0  0.000                              ! Cc-EO-C-C
GBL
```

```
Cc  4  O   4  C   15 H   0     0  0.000                              ! Cc-EO-C-H
GBL
O   11 Cc  2  O   10 C   21    2  0.000    2.905                     ! Oc-C1-EO-
C alkyl carbonate
Cc  2  O  10  C   21 C   21    0  0.000                              ! C1-EO-C-C
alkyl carbonate
Cc  2  O  10  C   21 H   0     3  0.000   0.000   -0.600            ! C1-EO-C-H
from PEO for alkyl carbonate
O   10 C  21  C   21 O   10    4  5.046   0.393   -0.015  0.772     ! EO-C-C-EO
in alkyl carbonates
*
*  Out-of-plain deformations for Lp
*  one must specify all charge types, and K(kcal/mol)
*
O   4   Cc  1   O   4  O  3           51.8        ! EC,transfered from
j.phys.chem.a.2003,107.7552
C  17   Cc  5   C  17  O  7           51.8        ! DMK,transfered from
j.phys.chem.a.2003,107.7552
O   1   Cc  2   O   1  O  7           51.8        ! DMC:transfered from
j.phys.chem.a.2003,107.7552
C  19   Cc  4   O   4  O  3           38.0        ! GBL from j.phys.chem.b 2004,
108,17990
O  11   Cc  2   O  11  O 10           38.8        ! alkyl carbonage from GBL
Cg  1   Cg  1   Cg  1  Cg 1           80.0        ! in graphite (guess)
end
```

*** Additional notes concerning input labels (atom types)
in EC,PC,DMC carbonyl oxygen and carbon atoms should be labeled Oc and Cc: ether ox -Oc too
in acetone (DMK) carbonyl carbone Cc, carbonyl oxygen in acetone is Oa
in gamma-BL (GBL) Oc=Cc-Obl are the special types, the other atoms have generic labels C, H,O
in EDC and MMC (alkyl carbonates) all carbons and oxygen atoms are labeled Cc and Oc respectively except for the carbonyl carbon that should be labeled C1

List of Abbreviations:
POM - poly(oxymethylene)
PEO - poly(ethylene oxide)
PTMO - poly(trimethylene oxide)
PPO - poly(propylene oxide)
DME - 1,2-dimethoxyethane (PEO oligomer)
DMP - 1,2-dimethoxypentane (PPO oligomer)
DMM - dimethoxyethane
DDE - 1,3-dimethoxydimethylether
EC   - ethylene carbonate
PC   - propylene carbonate
DMC - dimethyl carbonate
DMK - dimethyl ketone (acetone)
DMA - dimethyl amine
GBL - gamma butyrolactone
PTFE - poly(tetrafluoroethylene)
TFSI - bis(trifluorosulfa amide)
TFSIether- O-CH2-CF2-SO2-N-SO2-CF3
EDC - ethylene dicarbonate CO3CH2CH2CO3 (2-) (SEI layer product)
MMC - monomethyl carbonate CO3CH3 (-) (half of EDC)